

FLOWING GRANULAR MATERIALS AND THE MAXWELL-BOLTZMANN VELOCITY DISTRIBUTION

Edward J. Boyle
National Energy Technology Laboratory
3610 Collins Ferry Road
Morgantown, West Virginia 26507-0880

ABSTRACT

The single-granule velocity distribution function is shown to be Maxwell-Boltzmann for hard-sphere granular flows at steady-state exhibiting no gradients and absent a body-force. This is accomplished by approximating the two-granule velocity distribution function as the product of two single-granule velocity distribution functions and a correlating function and by applying to a canonical ensemble a function analogous to Boltzmann's H-function.

NOMENCLATURE

| | | | |
|---------------------------------|---|---------------------|--------------------------|
| C | constant of integration | m | granule mass |
| C_1 | vector of integration constants | n | granule number density |
| K | unit spatial vector, inverse collision | r | granule position |
| N | number of granules in a system | t | time |
| V | volume of a system | v | granule velocity |
| V | granule velocity, inverse collision | $\langle v \rangle$ | continuum velocity |
| X | body force | x,y,z | Cartesian coordinates |
| a | constant | Δt | instrument response time |
| c | constant of integration | Ψ | flow property |
| e_j | unit spatial vector in direction j | Σ | summation |
| e_r | restitution coefficient | Θ | granular temperature |
| $f(r, v_1, t)$, f | single-granule velocity distribution function | κ | Lagrange multiplier |
| $f^2(r, v_1, v_2, v_2)$, f^2 | two-granule velocity distribution function | ψ | granule property |
| $h(k, v_1, v_2)$, h | correlating function | ρ | continuum mass density |
| j | x, y, or z index | σ | granule diameter |
| k | unit spatial vector | μ | Lagrange multiplier |

INTRODUCTION

From power production to catalysis from cereal handling to chemical and pharmaceuticals manufacturing, granular materials are an important part of the economy. Accurately knowing how they move would allow for

tremendous savings in their processing. Since the work of Lun et al. (1984), the kinetic theory of gases (Chapman and Cowling, 1970) has been applied to predict the continuum properties of flowing granular materials. In using the kinetic theory of gases, the assumption has been that the steady-state distribution of velocities for granular flows that have no gradients is Maxwell-Boltzmann, the same as a gas in equilibrium. This distribution becomes the zeroth-order term in an expansion to predict the flow properties of shearing granular materials. The problem is that granules suffer inelastic collisions, whereas the usual development for gases (Chapman and Cowling, 1970; Hirshfelder et al., 1954; McQuarrie, 1973) considers only energy-conserving elastic collisions. Goldhirsh and Sela (1996) resolved this by using the Maxwell-Boltzmann distribution for elastic collisions as the zeroth-order term. This work presents a development indicating that the velocity distribution of even very inelastic granules is Maxwell-Boltzmann for steady-state flows exhibiting no gradients.

MODEL DEVELOPMENT

Imagine a canonical ensemble composed of a great number of macroscopically identical, closed systems. Each system has the same number of spherical granules N all with the same mass m and diameter σ . Let the mass of each spherical granule be concentrated at its center so that rotational degrees of freedom are ignored. Each system is enclosed within volume V , which is very large compared to its area so that boundary conditions are not considered. As time passes each system evolves according to Newton's Laws of Motion; granules collide inelastically and transform their kinetic energy into thermal energy. Because that thermal energy cannot be transformed back into kinetic energy, it is considered lost to the system. Thermal energy is replaced by kinetic energy transmitted through the walls of the system from a surrounding bath so large that it maintains a constant granular temperature Θ . Granular temperature is proportional to the kinetic energy of random motion. At any time, the macroscopic state of each system is characterized by N , V , and Θ .

Introduce the single-granule velocity distribution function $f(r, v_1, t)$ defined so that the most likely number of granules in any one selected system that has a velocity within dv_1 of v_1 and whose center is within dr of r during time Δt of t is $f(r, v_1, t) dr dv_1$. Practically, the time interval Δt is the largest time needed to replace kinetic energy lost by a collision, the time long enough for a representative number of granules to visit the subvolume at r , or the response time of a flow measurement device.

The evolution of average mass, momentum, and kinetic energy characterizes flows. Since each of these depends on the single-granule velocity distribution function, a description of flow is possible when the time rate of change of f is known,

$$\frac{d \Psi(r, t)}{dt} = \int_{-\infty}^{\infty} \psi(v_1) \frac{d f(r, v_1, t)}{dt} dv_1, \quad (1)$$

where $\psi(v_1)$ represents mass, momentum, or kinetic energy for a single representative granule, and $\Psi(r, t)$ is its average value within the flow. The time evolution of f is zero unless a collision occurs. A forward collision changes v_1 to another velocity v_1' , whereas an inverse collision changes it from some other velocity V_1 to v_1 .

For granules, mass and momentum are conserved during a collision, but kinetic energy is not. A simple model that takes into account the dissipation of kinetic energy into thermal energy whenever granules collide is one in which the granules bounce back with a relative velocity along their line of centers that is less than their pre-collision value (Jenkins and Savage, 1983). For forward and inverse collisions, respectively, the expressions are

$$e_R \mathbf{k} \cdot (v_2 - v_1) = -\mathbf{k} \cdot (v_2' - v_1') \quad \text{and} \quad e_R \mathbf{K} \cdot (V_2 - V_1) = -\mathbf{K} \cdot (v_2 - v_1) = \mathbf{k} \cdot (v_2 - v_1), \quad (2)$$

where the restitution coefficient e_R is a constant material property with a value between zero and one; v_2 and V_2 are the respective velocities of the striking granule for the forward and inverse collisions; and \mathbf{k} and \mathbf{K} are unit vectors that point in opposite directions from r to the center of their respective striking granule. The relationships among the variables describing the before and after of an inverse collision are

$$\begin{aligned} V_1 &= v_1 + \frac{1}{2} \frac{(1+e_R)}{e_R} \{ \mathbf{k} \cdot (v_2 - v_1) \} \quad \mathbf{k} = v_1 - \frac{1}{2} (1+e_R) \{ \mathbf{K} \cdot (V_2 - V_1) \} \mathbf{K} \\ V_2 &= v_2 - \frac{1}{2} \frac{(1+e_R)}{e_R} \{ \mathbf{k} \cdot (v_2 - v_1) \} \quad \mathbf{k} = v_2 + \frac{1}{2} (1+e_R) \{ \mathbf{K} \cdot (V_2 - V_1) \} \mathbf{K} \end{aligned} \quad (3)$$

By squaring and summing the expressions in Eq. (3) and applying Eq. (2), the change in the kinetic energy associated with an inverse collision is

$$0 = \frac{m}{2} (v_1^2 - V_1^2) + \frac{m}{2} (v_2^2 - V_2^2) + \frac{m}{4} \left([K \cdot (V_2 - V_1)]^2 - [k \cdot (v_2 - v_1)]^2 \right). \quad (4)$$

The Boltzmann equation describes the time rate of change in f in terms of forward and inverse collisions. For granules it is

$$\begin{aligned} \frac{df(r, v_1, t)}{dt} &= \frac{\partial f}{\partial t} + \nabla_r f \cdot v_1 + \nabla_{v_1} f \cdot \frac{X}{m} \\ &= -\sigma^2 \int_{k \cdot (v_2 - v_1) < 0} \int_{-\infty}^{\infty} \left(\frac{1}{c_R^2} f^2(r - \sigma k, V_2, r, V_1, t) - f^2(r + \sigma k, v_2, r, v_1, t) \right) \{ k \cdot (v_2 - v_1) \} dk dv_2, \end{aligned} \quad (5)$$

where X is a body force and f^2 is the two-granule velocity distribution function stating the likelihood that any two granules are respectively located at two points in space with two velocities (Goldhirsh and Sela, 1996). Equation (5) becomes the Boltzmann equation for a hard sphere gas by setting c_R to one, by closing it using Boltzmann's molecular chaos assumption to approximate the two-granule velocity distribution function as the product of two single-granule velocity distribution functions, and by requiring the spatial gradients of the flow to be small relative to the molecular diameter.

The time rate of change of any continuum property $\Psi(r, t)$ of a flowing gas is described by Enskog's general equation of change for molecular property $\psi(v)$. It is derived by multiplying the Boltzmann equation by $\psi(v)$, integrating over all v , and exploiting two symmetries (McQuarrie, 1973). The same can be done for granular flows because the two symmetrizing steps are a consequence of integrating over all v_1 as well as all v_2 , and are not affected by the restitution coefficient. The first symmetrizing step is recognizing that the velocity of the granule at r can be labeled either 1 or 2. The second step is recognizing that every collision involving a granule at r is both a forward collision and an inverse collision. Enskog's general equation of change for flowing granules is

$$\begin{aligned} \frac{d\Psi(r, t)}{dt} &= -\frac{\sigma^2}{4} \int_{k \cdot (v_2 - v_1) < 0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\psi(v_1) + \psi(v_2) - \psi(V_1) - \psi(V_2)] \times \\ &\quad \left(\frac{1}{c_R^2} f^2(r - \sigma k, V_2, r, V_1, t) - f^2(r + \sigma k, v_2, r, v_1, t) \right) \{ k \cdot (v_2 - v_1) \} dk dv_2 dv_1. \end{aligned} \quad (6)$$

The goal is to determine f for a steady-state granular flow exhibiting no gradients and absent a body force. To proceed further, and in contrast to the molecular chaos assumption, f^2 is approximated as the product of two single-particle velocity distribution functions f and a correlating function h that depends upon k , v_1 , and v_2 for the forward collision and upon K , V_1 , and V_2 for the inverse collision,

$$\begin{aligned} \frac{1}{c_R^2} f^2(r - \sigma k, V_2, r, V_1, t) - f^2(r + \sigma k, v_2, r, v_1, t) = \\ \frac{1}{c_R^2} h(K, V_1, V_2) f(r - \sigma k, V_2, t) f(r, V_1, t) - h(k, v_1, v_2) f(r + \sigma k, v_2, t) f(r, v_1, t). \end{aligned} \quad (7)$$

The next step is to apply Enskog's general equation for change to the steady-state, no gradients and no body-force case. In analogy with the Boltzmann H-function for the micro canonical ensemble (McQuarrie, 1973), the relevant property to use for the canonical ensemble is

$$\psi(v) = \ln[f(v)] + \frac{1}{2} \frac{mv^2}{m\Theta} \quad \text{or} \quad \Psi = \int_{-\infty}^{\infty} \left(\ln[f(v_1)] + \frac{1}{2} \frac{mv_1^2}{m\Theta} \right) f(v_1, t) dv_1. \quad (8)$$

Using this property, Enskog's general equation for change, Eq. (6), becomes

$$\begin{aligned}
\frac{d\mathcal{P}}{dt} = & -\frac{\sigma^2}{4} \int_{\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) < 0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\frac{m\mathbf{v}_1^2 + m\mathbf{v}_2^2 - m\mathbf{V}_1^2 - m\mathbf{V}_2^2}{2m\Theta} \right] \times \\
& \left(\frac{1}{e_R^2} h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2) f(\mathbf{V}_2, t) f(\mathbf{V}_1, t) - h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2) f(\mathbf{v}_2, t) f(\mathbf{v}_1, t) \right) \{ \mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) \} d\mathbf{k} dv_2 dv_1 \\
& - \frac{\sigma^2}{4} \int_{\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) < 0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \{ \ln[f(\mathbf{v}_1)] + \ln[f(\mathbf{v}_2)] - \ln[f(\mathbf{V}_1)] - \ln[f(\mathbf{V}_2)] \} \times \\
& \left(\frac{1}{e_R^2} h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2) f(\mathbf{V}_2, t) f(\mathbf{V}_1, t) - h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2) f(\mathbf{v}_2, t) f(\mathbf{v}_1, t) \right) \{ \mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) \} d\mathbf{k} dv_2 dv_1. \tag{9}
\end{aligned}$$

To the braces in the second term on the right side of Eq. (9) add $\ln \frac{e_R^2 h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2)}{h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2)}$ and subtract it from the brackets in

the first term,

$$\begin{aligned}
\frac{d\mathcal{P}}{dt} = & -\frac{\sigma^2}{4} \int_{\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) < 0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\frac{m\mathbf{v}_1^2 + m\mathbf{v}_2^2 - m\mathbf{V}_1^2 - m\mathbf{V}_2^2}{2m\Theta} - \ln \frac{e_R^2 h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2)}{h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2)} \right] \times \\
& \left(\frac{1}{e_R^2} h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2) f(\mathbf{V}_2, t) f(\mathbf{V}_1, t) - h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2) f(\mathbf{v}_2, t) f(\mathbf{v}_1, t) \right) \mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) d\mathbf{k} dv_2 dv_1 \\
& - \frac{\sigma^2}{4} \int_{\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) < 0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ \ln[f(\mathbf{v}_1)] + \ln[f(\mathbf{v}_2)] - \ln[f(\mathbf{V}_1)] - \ln[f(\mathbf{V}_2)] + \ln \frac{e_R^2 h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2)}{h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2)} \right\} \times \\
& \left(\frac{1}{e_R^2} h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2) f(\mathbf{V}_2, t) f(\mathbf{V}_1, t) - h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2) f(\mathbf{v}_2, t) f(\mathbf{v}_1, t) \right) \mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) d\mathbf{k} dv_2 dv_1. \tag{10}
\end{aligned}$$

The first term on the right side is zero as long as

$$\ln \frac{e_R^2 h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2)}{h(\mathbf{K}, \mathbf{V}_1, \mathbf{V}_2)} = \frac{m\mathbf{v}_1^2 + m\mathbf{v}_2^2 - m\mathbf{V}_1^2 - m\mathbf{V}_2^2}{2m\Theta} = -\frac{1}{4\Theta} \left([\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)]^2 - [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]^2 \right). \tag{11}$$

This will be shown to be the case. For now assume that the first term is zero, and notice that Eq. (11) implies that a solution is sought in which the argument of the correlating function is $\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)$; $h(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2) = h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1))$.

The integrand appearing in the second term of the right side of Eq. (10) can be written as

$$\ln \frac{f^2(\mathbf{v}_2, \mathbf{v}_1, t)}{\frac{1}{e_R^2} f^2(\mathbf{V}_2, \mathbf{V}_1, t)} \left(\frac{1}{e_R^2} f^2(\mathbf{V}_2, \mathbf{V}_1, t) - f^2(\mathbf{v}_2, \mathbf{v}_1, t) \right) \{ \mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1) \}. \tag{12}$$

Regardless if $f^2(\mathbf{V}_2, \mathbf{V}_1, t)/e_R^2 > f^2(\mathbf{v}_2, \mathbf{v}_1, t)$ or $f^2(\mathbf{V}_2, \mathbf{V}_1, t)/e_R^2 < f^2(\mathbf{v}_2, \mathbf{v}_1, t)$, this integrand is everywhere positive. Consequently, the time rate of change in \mathcal{P} is always negative. Since \mathcal{P} is bounded, its rate of change eventually becomes zero as does the remaining integral on the right side of Eq. (10). This is possible only if $f^2(\mathbf{V}_2, \mathbf{V}_1)/e_R^2 = f^2(\mathbf{v}_2, \mathbf{v}_1)$ for all \mathbf{v}_1 and \mathbf{v}_2 . Accordingly, for the steady-state flow that exhibits no gradients and no body force, the

Boltzmann equation, Eq. (5), simplifies to

$$\frac{1}{e_R^2} h(\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)) f(\mathbf{V}_2) f(\mathbf{V}_1) = h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)) f(\mathbf{v}_2) f(\mathbf{v}_1) \quad , \quad \text{or}$$

$$0 = \ln(h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1))) + \ln(f(\mathbf{v}_2)) + \ln(f(\mathbf{v}_1)) - \ln(h(\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1))) - \ln(f(\mathbf{V}_2)) - \ln(f(\mathbf{V}_1)) + \ln(e_R^2) \quad . \quad (13)$$

The derivation of f as presented by Kennard (1938) is followed. The functions f and h are found by requiring that they make Eq. (13) stationary under the constraints of mass, momentum, kinetic energy, and line-of-centers velocity changes for an inverse collision. By inspection, the objective function in Eq. (13) depends on fourteen variables. Six are held constant by considering only those inverse collisions with constant \mathbf{V}_1 and \mathbf{V}_2 . The independence of the three components of \mathbf{v}_2 is eliminated by explicitly considering the differential changes in the three momentum equations, $m\mathbf{v}_1 + m\mathbf{v}_2 - m\mathbf{V}_1 - m\mathbf{V}_2 = 0$,

$$m \, dv_{1x} + m \, dv_{2x} = 0, \quad m \, dv_{1y} + m \, dv_{2y} = 0, \quad \text{and} \quad m \, dv_{1z} + m \, dv_{2z} = 0, \quad \text{or} \quad dv_{2j} = -dv_{1j}, \quad j=x,y,z \quad . \quad (14)$$

Variations in the five remaining variables express the differential change in the kinetic energy, Eq. (4),

$$0 = \sum_{j=x,y,z} m(\mathbf{v}_{1j} - \mathbf{v}_{2j}) \, dv_{1j} + \frac{m}{2} [\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)] \, d[\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)] - \frac{m}{2} [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)] \, d[\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)] \quad , \quad (15)$$

the differential change in the relationship between the line-of-centers velocities associated with an inverse collision, Eq. (2),

$$0 = e_R \, d[\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)] - d[\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)] \quad , \quad (16)$$

and the variation in the objective function, Eq. (13),

$$0 = \sum_{j=x,y,z} \left(\frac{\partial \ln(f(\mathbf{v}_1))}{\partial v_{1j}} - \frac{\partial \ln(f(\mathbf{v}_2))}{\partial v_{2j}} \right) dv_{1j} + \frac{\partial \ln(h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)))}{\partial [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]} d[\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]$$

$$- \frac{\partial \ln(h(\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)))}{\partial [\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)]} d[\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)] \quad . \quad (17)$$

Lagrange's undetermined multiplier method is used to extremize the above variation under the constraints for the energy, Eq. (15) and the line-of-centers velocity, Eq. (16). The Lagrange multipliers are μ and κ ,

$$0 = \sum_{j=x,y,z} \left(\frac{\partial \ln(f(\mathbf{v}_1))}{\partial v_{1j}} - \frac{\partial \ln(f(\mathbf{v}_2))}{\partial v_{2j}} + \mu m(\mathbf{v}_{1j} - \mathbf{v}_{2j}) \right) dv_{1j}$$

$$+ \left(\frac{\partial \ln(h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1), e_R))}{\partial [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]} - \frac{\mu m}{2} [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)] - \kappa \right) d[\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]$$

$$- \left(\frac{\partial \ln(h(\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)))}{\partial [\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)]} - \frac{\mu m}{2} [\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)] - \kappa e_R \right) d[\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)] \quad . \quad (18)$$

Each of these five coefficients must be zero because $[\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]$, $[\mathbf{K} \cdot (\mathbf{V}_2 - \mathbf{V}_1)]$, and the components of \mathbf{v}_1 can vary independently of each other.

To start, set the coefficient of $d[\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]$ to zero. It becomes

$$\frac{\partial \ln(h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1), e_R))}{\partial [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]} = \frac{\mu m}{2} [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)] + \kappa \quad , \quad (19)$$

which is integrated to yield

$$\ln(h(\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1))) = \frac{\mu m}{4} [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]^2 + \kappa [\mathbf{k} \cdot (\mathbf{v}_2 - \mathbf{v}_1)] + c \quad . \quad (20)$$

Likewise the coefficient for $d[K \cdot (V_2 - V_1)]$ is set to zero and integrated to yield

$$\ln(h(K(V_2 - V_1))) = \frac{\mu m}{4} [K(V_2 - V_1)]^2 + \kappa e_R [K(V_2 - V_1)] + C \quad (21)$$

Now set to zero the coefficient for dv_{1x} in Eq. (18),

$$\frac{\partial \ln(f(v_1))}{\partial v_{1x}} - \frac{\partial \ln(f(v_2))}{\partial v_{2x}} = -\mu m (v_{1x} - v_{2x}) \quad (22)$$

Differentiating again by either v_{1y} or v_{1z} yields $\frac{\partial^2 \ln(f(v_1))}{\partial v_{1y} \partial v_{1x}} = 0$, because $f(v_2)$ is independent of the components of

v_1 . This indicates that $\frac{\partial \ln(f(v_1))}{\partial v_{1x}}$ depends only upon v_{1x} . Similarly, every first derivative of either $f(v_1)$ or $f(v_2)$ is a function solely of the variable named in the derivative. Differentiating Eq. (22), by v_{1x} yields

$$\frac{\partial^2 \ln(f(v_1))}{\partial v_{1x}^2} = -\mu m \quad (23)$$

which is twice integrated, knowing that the first derivative depends on v_{1x} alone, to obtain

$$\ln(f(v_1)) = \frac{-\mu m}{2} v_{1x}^2 + C_{1x} v_{1x} + C_{yz} \quad (24)$$

where C_{1x} is a constant and C_{yz} may be a function of v_{1y} and v_{1z} . Differentiating this twice with respect to v_{1y} yields

$$\frac{\partial^2 \ln(f(v_1))}{\partial v_{1y}^2} = \frac{\partial^2 C_{yz}}{\partial v_{1y}^2} \quad (25)$$

The coefficient multiplying dv_{1y} in Eq. (18) is set to zero and differentiated with respect to v_{1y} to yield

$$\frac{\partial^2 \ln(f(v_1))}{\partial v_{1y}^2} = -\mu m \quad (26)$$

Comparing the two expressions for $\frac{\partial^2 \ln(f(v_1))}{\partial v_{1y}^2}$, Eq. (25) and Eq. (26), indicates that

$$C_{yz} = \frac{-\mu m}{2} v_{1y}^2 + C_{1y} v_{1y} + C_z \quad (27)$$

where C_{1y} is a constant and C_z may be a function of v_{1z} . This expression for C_{yz} is substituted into Eq. (24),

$$\ln(f(v_1)) = -\frac{\mu m}{2} v_{1x}^2 - \frac{\mu m}{2} v_{1y}^2 + C_{1x} v_{1x} + C_{1y} v_{1y} + C_z \quad (28)$$

To evaluate C_z twice differentiate Eq. (28) with respect to v_{1z} and subtract from it the result obtained by setting the coefficient of dv_{1z} in Eq. (18) to zero and differentiating it with respect to v_{1z} . The result is

$$\frac{\partial^2 C_z}{\partial v_{1z}^2} = -\mu m, \text{ or } C_z = -\frac{\mu m}{2} v_{1z}^2 + C_{1z} v_{1z} + C_1 \quad (29)$$

Both C_{1z} and C_1 are constants. With that, Eq. (28) becomes

$$\begin{aligned} \ln(f(v_1)) &= -\frac{\mu m}{2} v_{1x}^2 - \frac{\mu m}{2} v_{1y}^2 - \frac{\mu m}{2} v_{1z}^2 + C_{1x} v_{1x} + C_{1y} v_{1y} + C_{1z} v_{1z} + C_1 \\ &= -\frac{\mu m}{2} v_1^2 + C_1 \cdot v_1 + C_1 \end{aligned} \quad (30)$$

The Lagrange multiplier μ and the constants $C_1 = C_{1x}e_x + C_{1y}e_y + C_{1z}e_z$ and C_1 are evaluated by requiring that the averages of mass density and velocity be their measured values for the continuum and by requiring that the variance in the velocity be related to the granular temperature. Following McQuarrie (1973), define $\ln(a) = C_1 + \frac{C_1 \cdot C_1}{2 \mu m}$ and express $\ln(f(v_1))$ as

$$\ln(f(v_1)) = \ln(a) - \frac{\mu m}{2} \left(v_1 - \frac{C_1}{\mu m} \right)^2, \quad \text{or} \quad f(v_1) = a \exp \left\{ -\frac{\mu m}{2} \left(v_1 - \frac{C_1}{\mu m} \right) \cdot \left(v_1 - \frac{C_1}{\mu m} \right) \right\} \quad (31)$$

The mass density is

$$\rho = m \int f(v_1) dv_1 = m a \int \exp \left\{ -\frac{\mu m}{2} \left(v_1 - \frac{C_1}{\mu m} \right) \cdot \left(v_1 - \frac{C_1}{\mu m} \right) \right\} dv_1 = m a \left(\frac{2\pi}{\mu m} \right)^{\frac{3}{2}} \quad (32)$$

The component of the average velocity in the x direction is

$$\begin{aligned} \langle v_x \rangle &= \frac{m a}{\rho} \int v_{1x} f(v_1) dv_1 = \frac{m a}{\rho} \int v_{1x} e^{-\frac{\mu m}{2} \left(v_{1x} - \frac{C_{1x}}{\mu m} \right)^2} dv_{1x} \iint e^{-\frac{\mu m}{2} \left(v_{1y} - \frac{C_{1y}}{\mu m} \right)^2 - \frac{\mu m}{2} \left(v_{1z} - \frac{C_{1z}}{\mu m} \right)^2} dv_{1y} dv_{1z} \\ &= \frac{C_{1x}}{\mu m} \end{aligned} \quad (33)$$

The other continuum velocity components together with $\langle v_x \rangle$ yield $\langle v \rangle = (C_{1x}e_x + C_{1y}e_y + C_{1z}e_z) / (\mu m)$. Granular temperature is related to the variance of the velocity,

$$\begin{aligned} \frac{3}{2} \Theta &= \frac{1}{2} \langle (v_1 - \langle v \rangle)^2 \rangle = \frac{1}{2\rho} \int (v_1^2 - \langle v \rangle^2) f(v_1) dv_1 = \frac{1}{2\rho} \int \sum_{j=x,y,z} \left(v_{1j}^2 - \left(\frac{C_{1j}}{\mu m} \right)^2 \right) f(v_1) dv_1 \\ &= \frac{3}{2 \mu m} \end{aligned} \quad (34)$$

These results, $\mu m = \frac{1}{\Theta}$, $\langle v_j \rangle = \frac{C_{1j}}{\mu m}$, and $a = \frac{\rho}{m} \left(\frac{1}{2\pi\Theta} \right)^{\frac{3}{2}} = n \left(\frac{1}{2\pi\Theta} \right)^{\frac{3}{2}}$, are substituted into Eq. (31) to yield the Maxwell-Boltzmann velocity distribution,

$$f(v_1) = a e^{-\frac{\mu m}{2} \left(v_1 - \frac{C_1}{\mu m} \right) \cdot \left(v_1 - \frac{C_1}{\mu m} \right)} = n \left(\frac{1}{2\pi\Theta} \right)^{\frac{3}{2}} e^{-\frac{1}{2\Theta} (v_1 - \langle v \rangle)^2}, \quad \text{and} \quad f(V_1) = n \left(\frac{1}{2\pi\Theta} \right)^{\frac{3}{2}} e^{-\frac{1}{2\Theta} (V_1 - \langle v \rangle)^2}, \quad (35)$$

where n is granule number density. Likewise

$$f(v_2) = n \left(\frac{1}{2\pi\Theta} \right)^{\frac{3}{2}} e^{-\frac{1}{2\Theta} (v_2 - \langle v \rangle)^2} \quad \text{and} \quad f(V_2) = n \left(\frac{1}{2\pi\Theta} \right)^{\frac{3}{2}} e^{-\frac{1}{2\Theta} (V_2 - \langle v \rangle)^2} \quad (36)$$

These results are substituted into the objective function, Eq. (13), in order to evaluate the difference in the constants c and C from Eq. (20) and Eq. (21),

$$\begin{aligned}
0 &= \ln(h(k(v_2 - v_1))) - \ln(h(K(V_2 - V_1))) + \ln(f(v_1)) - \ln(f(V_1)) + \ln(f(v_2)) - \ln(f(V_2)) + \ln(e_r^2) \\
0 &= \frac{\mu}{2}(mv_1^2 + mv_2^2 - mV_1^2 - mV_2^2) + c - C + \frac{\mu m}{2}[(V_1 - \langle v \rangle)^2 - (v_1 - \langle v \rangle)^2] + \frac{\mu m}{2}[(V_2 - \langle v \rangle)^2 - (v_2 - \langle v \rangle)^2] + \ln(e_r^2) \\
0 &= c - C + \mu m [v_1 + v_2 - V_1 - V_2] \cdot \langle v \rangle + \ln(e_r^2) \quad \text{or} \quad C = c + \ln(e_r^2) \tag{37}
\end{aligned}$$

This result and $\mu=1/m\Theta$, Eq. (34), are substituted into Eq. (21) and Eq. (22) to yield

$$\begin{aligned}
\ln(h(k(v_2 - v_1))) &= \frac{1}{4\Theta} [k(v_2 - v_1)]^2 + \kappa [k(v_2 - v_1)] + c \quad \text{and} \\
\ln(h(K(V_2 - V_1))) &= \frac{1}{4\Theta} [K(V_2 - V_1)]^2 + \kappa e_r [K(V_2 - V_1)] + \ln(e_r^2) + c \tag{38}
\end{aligned}$$

The two expressions in Eq. (38) are combined to reproduce the remaining criterion for the objective function to be zero, namely that Eq. (11) is satisfied. Thus, the velocity distribution function for gradient-free, steady-state granular flows in the absence of a body force is Maxwell-Boltzmann.

SUMMARY

An approach is presented that indicates that the single-granule velocity distribution function for a primitive model granular flow at steady-state and absent a body force and gradients is Maxwell-Boltzmann, the same as a gas in equilibrium, and in agreement with the central limit theorem of statistics. The inelasticity of a granular collision is treated by causing the rebound velocity along the line of centers to be less than the incoming velocity; consequently, the ensemble is canonical and Enskog's general equation for change is applied to a function that is proportional to the Helmholtz free energy. For the Helmholtz free energy to obtain a stationary value, Boltzmann's molecular chaos assumption is replaced with a correlating function that depends on the relative velocity along the line of centers of the colliding granules. The Maxwell-Boltzmann velocity distribution then follows from Kennard's (1938) variational approach. These results are also applicable to hard-sphere gases by setting e_r to one and everywhere replacing Θ with $k_B T/m$, where k_B is Boltzmann's constant and T is absolute temperature.

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